

# Realizations of complex logic operations at the nanoscale

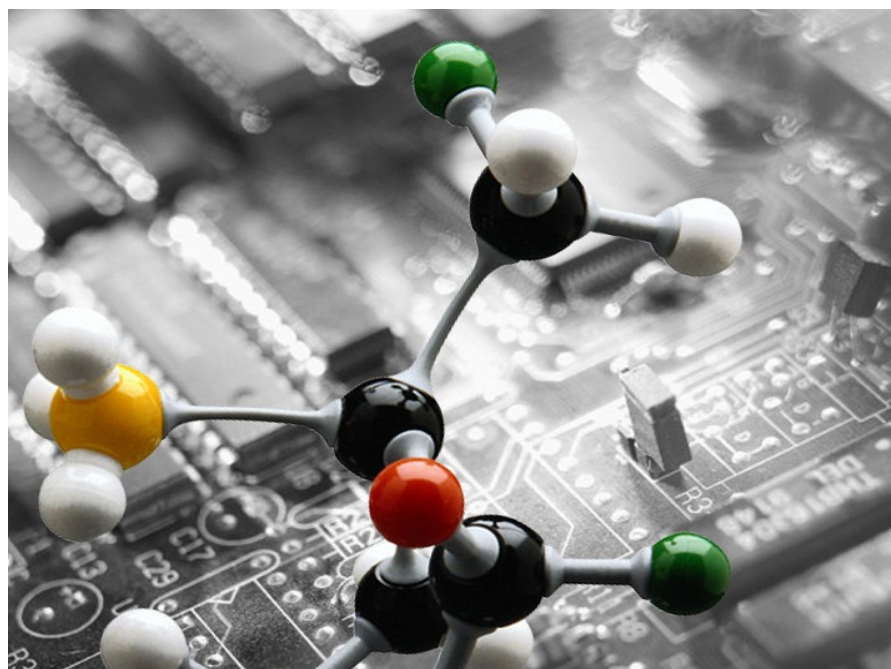
F. Remacle

University of Liège, Belgium

FP7 FET proactive Nano-ICT 215750 : New Functionalities

# MOLOC

MOLecular LOGic Circuits



# Objectives

Realize complex logic operations at the hardware level at the nanoscale

Beyond the switching paradigm :

- provide the foundation of a **Post-Boolean** approach
- provide new logic schemes that enables complex logic functions

Experimental realizations of

- logic circuits (Boolean) directly implemented at the hardware level
- multivalued logic circuits (ternary multiplier and ternary adder)
- search and identification function algorithm as a finite state machine

# Quasi classical approach

- encode Boolean or multi-valued variables in the discrete charge, energy or conformational states of confined molecular or nano systems.
- provide inputs as a selective perturbation that induces specific transitions between these states.
- processing of information is performed by the quantum dynamics of the multi state system.
- the outputs are a probe of the final states.

Different from quantum computing : no information is encoded into the phase of the wave function.

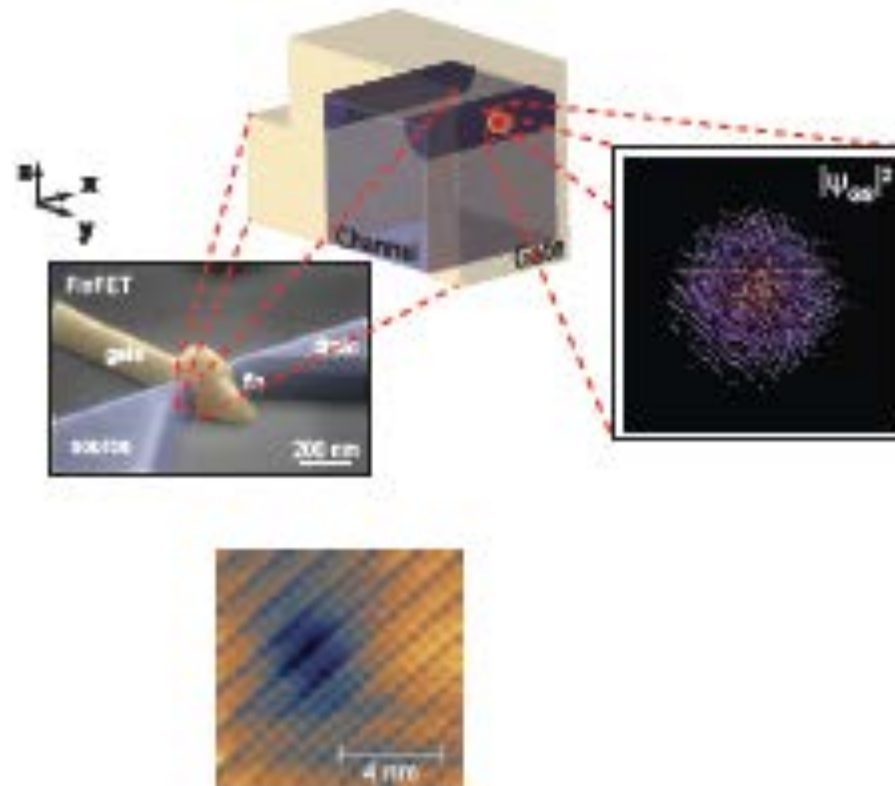
# Implementations of electrically addressed logic circuits at the hardware level

Transport through a single atom in a silicon transistor (SAT).

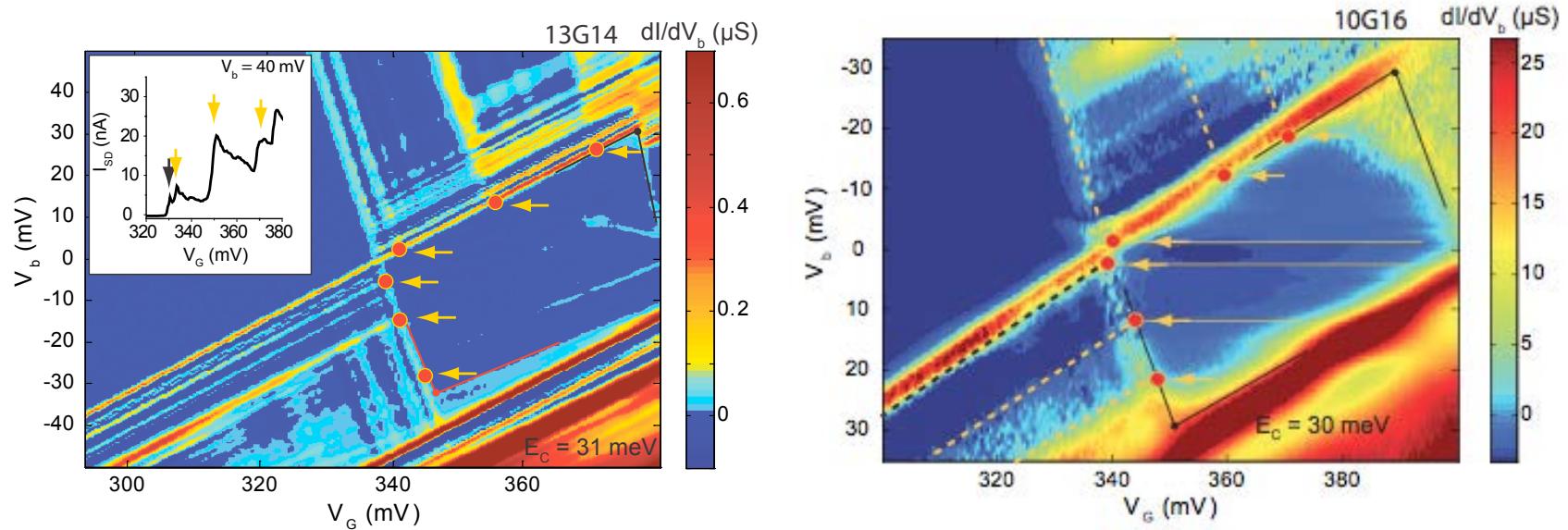
Sven Rogge



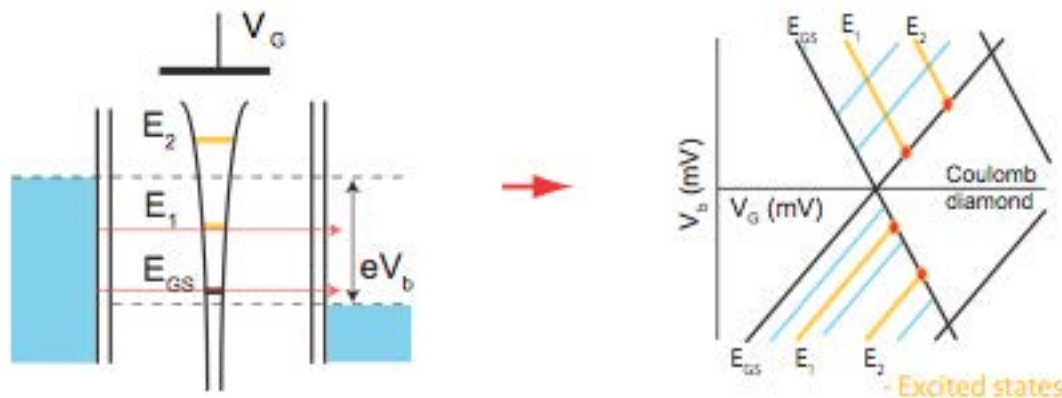
TU- Delft  
School of Physics & CQC<sup>2</sup>T  
University of New South Wales  
Australia



# Assignment of the level spectrum of the As dopant atom from the stability maps of a FinFET transistor

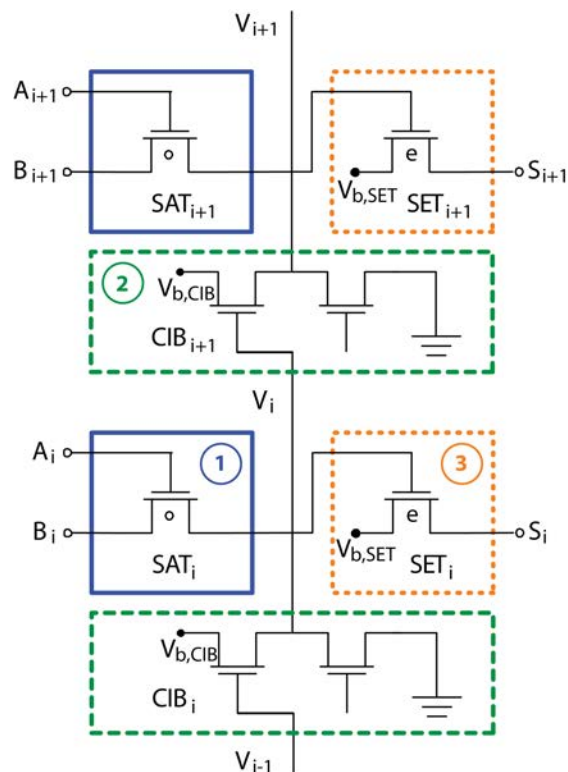


Excited electronic states of a given charge As dopant



Lansberger et al, Nature Physics, **4** , 656 (2008)

# Physical realization of a cascade of two full binary adders



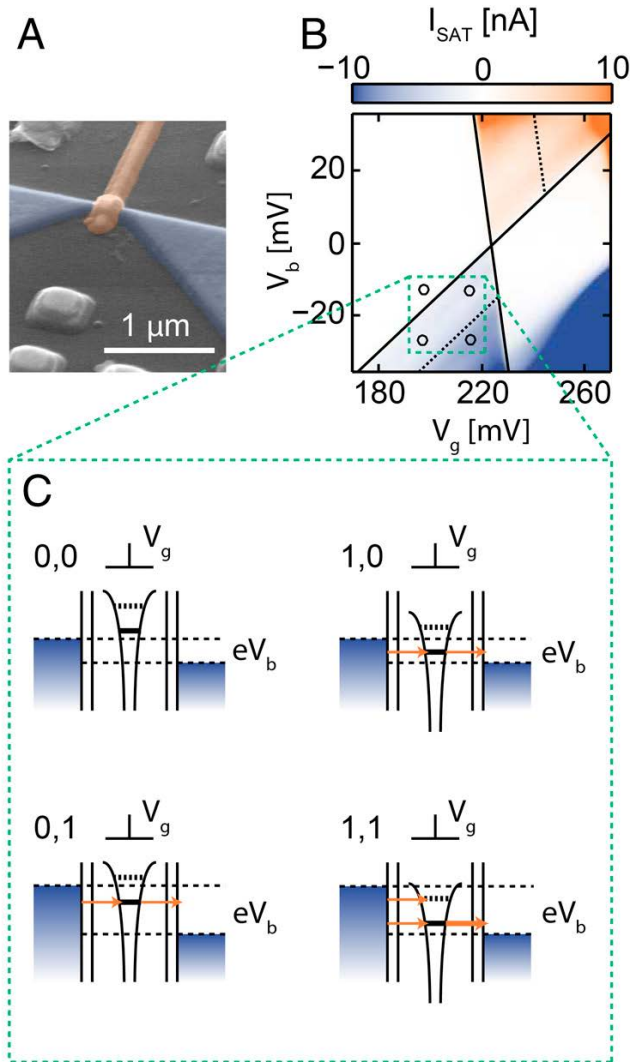
1. SAT : half addition  $A_i + B_i$
2. CIB : FET + load resistor :  
 $V_i$  is the arithmetic sum  $A_i + B_i + C_{i-1}$
3. A SET decodes the arithmetic sum to  
a Boolean variable

- multivalued logic scheme
- CMOS compatible
- scalable
- each full addition requires 4 transistors  
reduces the number of switches by a factor 7

J.A. Mol, J. Verduijn, R. D. Levine, F. Remacle and S. Rogge, PNAS, **108**, 13969 (2011).

M. Klein, G. P. Lansbergen, J. A. Mol, S. Rogge, R. D. Levine, and F. Remacle, ChemPhysChem. **10**: 162-173, 2009.

# Half addition performed by the SAT



- A and B are encoded as two values of  $V_b$  and  $V_g$
- depending on these values,
  - zero level (0,0) contribute
  - one level (0,1) and (1,0) to the
  - two levels (1,1) current

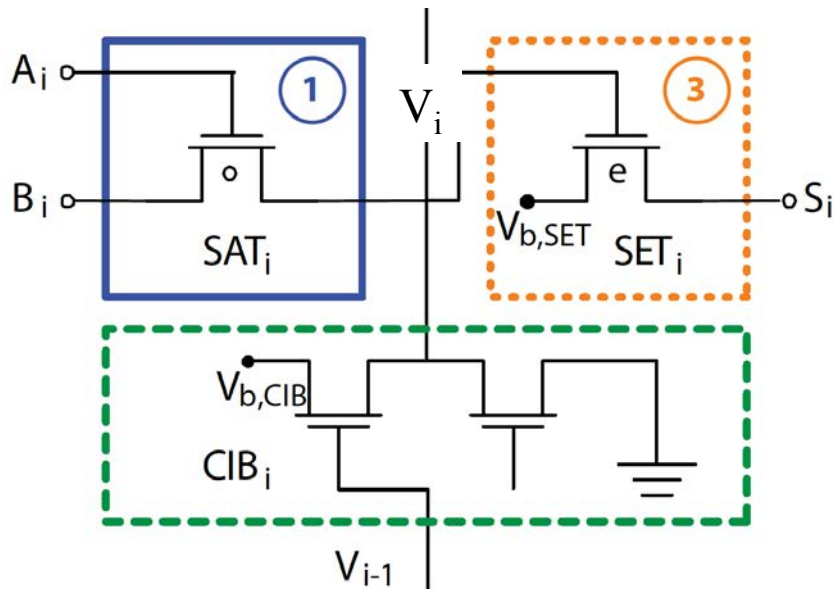
half addition

A	B	$C_{in}$	a.s.	$C_{out}$	S
0	0	0	0	0	0
0	1	0	1	0	1
1	0	0	1	0	1
1	1	0	2	1	0
0	0	1	1	0	1
0	1	1	2	1	0
1	0	1	2	1	0
1	1	1	3	1	1



## CIB and decoder to Boolean

$$V_i = A_i + B_i + V_{i-1}$$



SET<sub>i</sub> converts the a.s. to a Boolean signal. The conversion is implemented using the periodicity of the SET.  $V_i$  is applied to the gate of the SET and gives a current that corresponds to  $S_i$

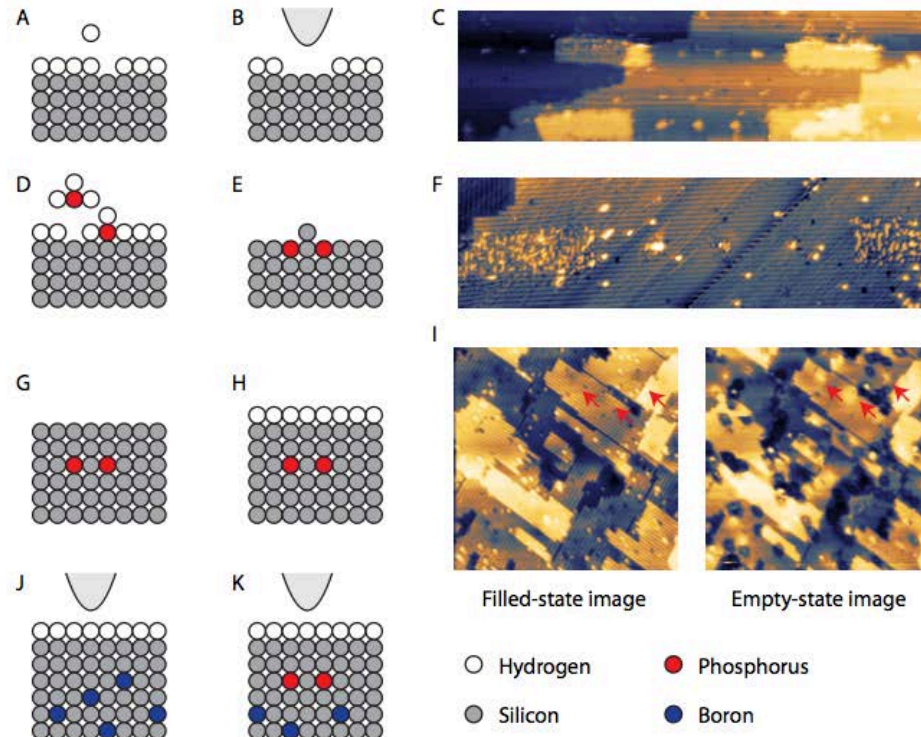
a.s is a four valued signal

- CIB : carry in buffer , made of
- a load resistor (converts  $I_{i-1}$  to  $V_{i-1}$ )
  - a carry in FET opened if the arithmetic sum,  $V_{i-1}$ , is larger than 1 ( $C_i = 1$ ).
  - provides gain

$A$	$B$	$C_{in}$	a.s.	$C_{out}$	$S$
0	0	0	0	0	0
0	1	0	1	0	1
1	0	0	1	0	1
1	1	0	2	1	0
0	0	1	1	0	1
0	1	1	2	1	0
1	0	1	2	1	0
1	1	1	3	1	1

# Perspective : engineer molecular structure in Silicon

## Interactions in molecular structures: dopant placement



## effective mass model for the two dopant molecule

$$H(t) = - \left[ \frac{\hbar^2}{2m_{\perp}} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{\hbar^2}{2m_{\parallel}} \frac{\partial^2}{\partial z^2} \right] + e\mathbf{F}(t) \cdot \mathbf{r} - \sum_{i=1}^2 \frac{e^2}{\epsilon_{\text{Si}} \sqrt{(x-x_i)^2 + y^2 + (z-z_i)^2}} + \sum_{i=1}^2 \frac{Qe^2}{\epsilon_{\text{Si}} \sqrt{(x-x_i)^2 + y^2 + (z-z_i)^2}} - \frac{Qe^2}{4\epsilon_{\text{Si}}z}$$

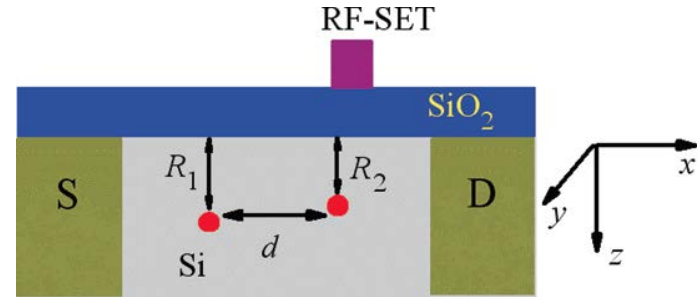
Time –dependent Hamiltonian is solved on a 3D grid

$$\begin{cases} m_{\perp} = 0.191m_e \\ m_{\parallel} = 0.916m_e \end{cases} \quad Q = (\epsilon_{\text{SiO}_2} - \epsilon_{\text{Si}}) / (\epsilon_{\text{SiO}_2} + \epsilon_{\text{Si}}) \quad \begin{cases} \epsilon_{\text{Si}} = 11.4 \\ \epsilon_{\text{SiO}_2} = 3.8 \end{cases}$$

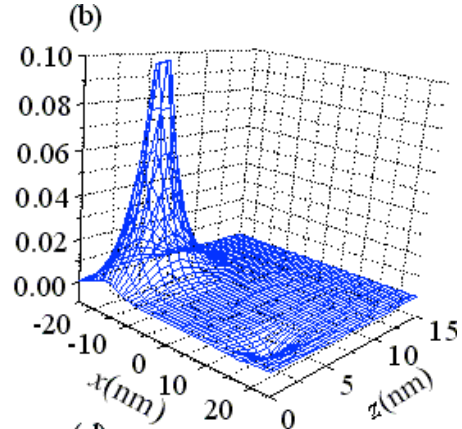
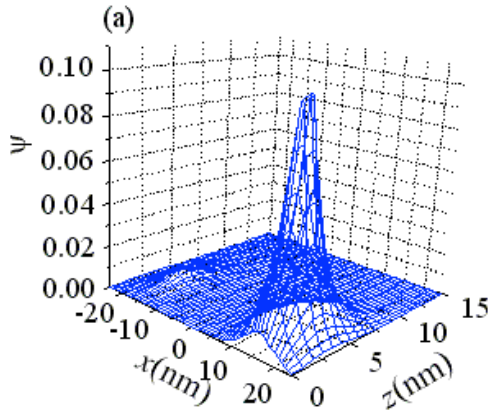
Y. Yan, J. A. Mol, J. Verduijn, S. Rogge, R. D. Levine, and F. Remacle, J. Phys. Chem. C **114**: 20380-20386, 2010.

# Control of the localization of the charge by a static gate field

hetero nuclear dopant molecule

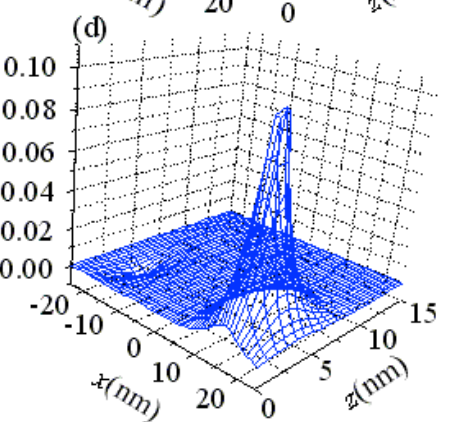
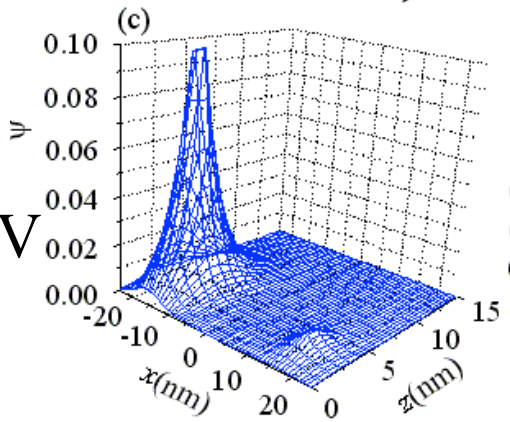


$$F_x = 0$$



GS

$$F_x = 0.01 \text{ kV}$$



First excited state

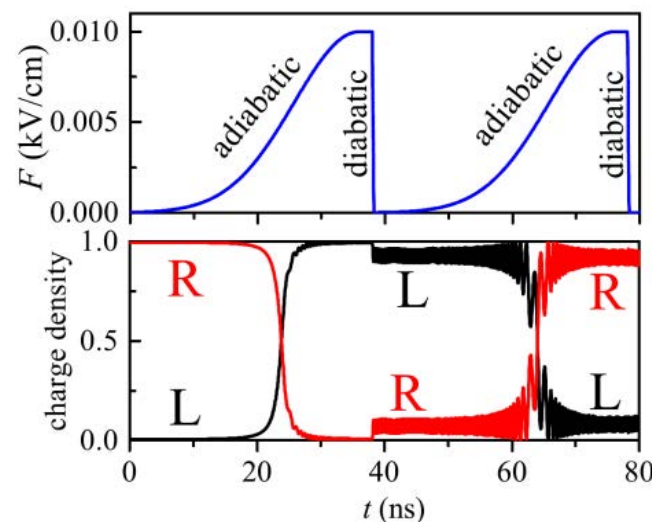
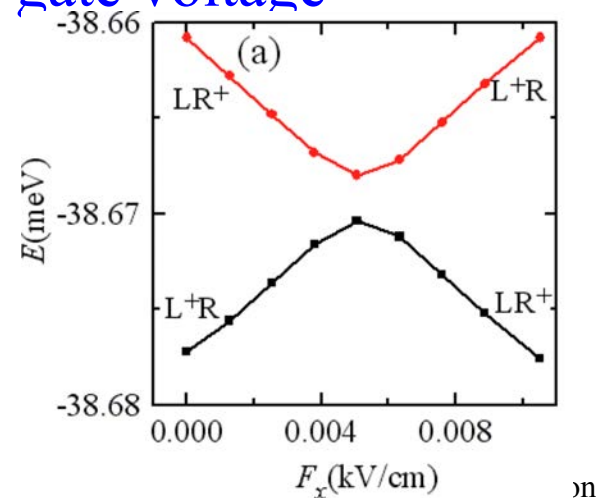
# Cyclable full adder implemented on dopant molecule addressed by a pulse gate voltage

first half addition

initial state	voltage pulse	XOR int sum	AND (c1)	INH
L+R (0)	0	L+R (0)	0	0
L+R (0)	1	LR+ (1)	0	1
LR+ (1)	0	LR+ (1)	0	0
LR+ (1)	1	L+R (0)	1	0

second half addition

int sum	voltage pulse	XOR final sum	AND (c2)	INH
L+R (0)	0	L+R (0)	0	0
L+R (0)	1	LR+ (1)	0	1
LR+ (1)	0	LR+ (1)	0	0
LR+ (1)	1	L+R (0)	1	0

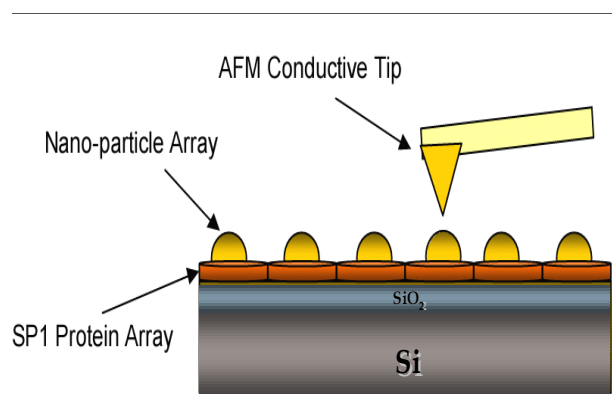


AND : charge on right at  $F_{\max}$   
 INH : charge on left at  $F_{\max}$

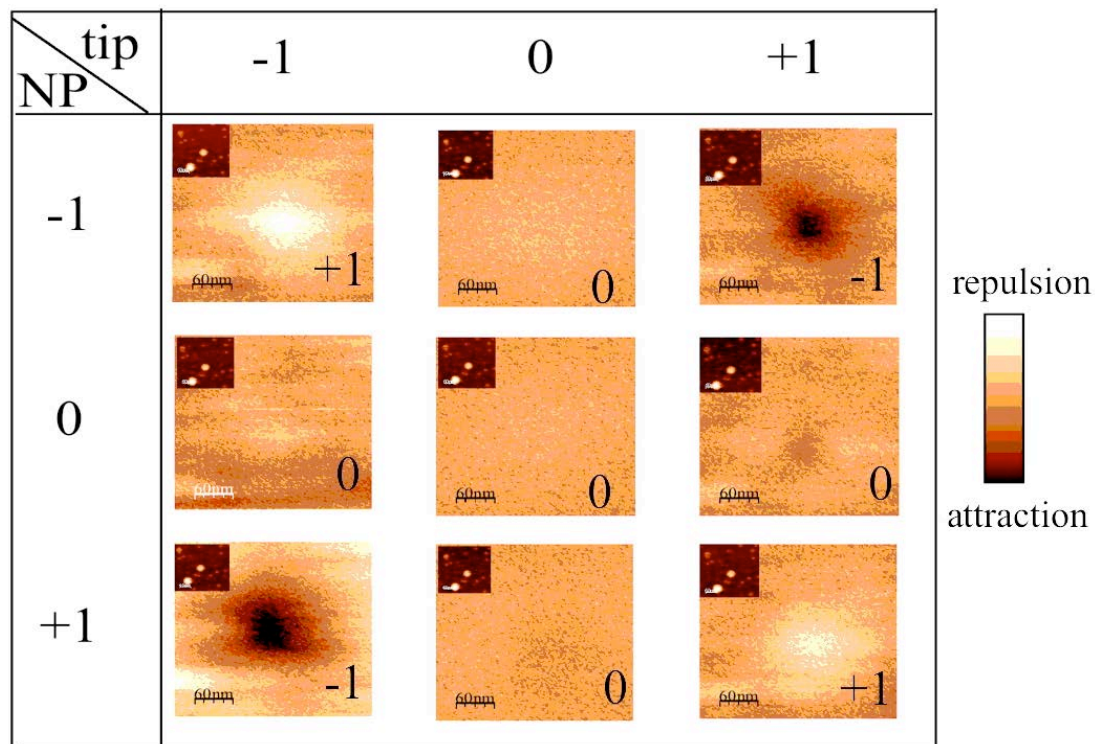
Y. Yan, J. A. Mol, J. Verduijn, S. Rogge, R. D. Levine, and F. Remacle, *J. Phys. Chem. C* **114**: 20380-20386, 2010.

# Multivalued logic : implementation of ternary logic circuits

## A ternary multiplier on a Si NP



scalable  
room temperature

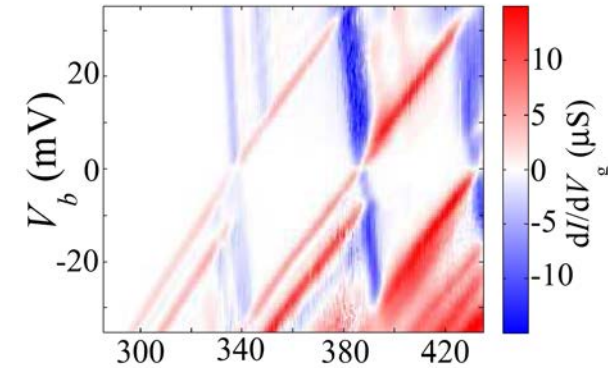


I. Medalsy, M. Klein, A. Heyman, O. Shoseyov, F. Remacle, R. D. Levine, and D. Porath, Nature Nanotechnology **5**: 451-457, 2010.

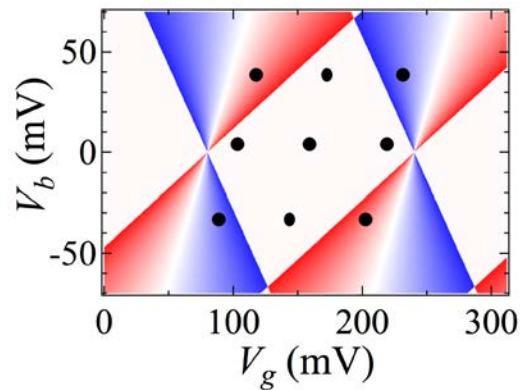
# Ternary multiplier on a single dopant atom in a transistor

multi	-1	0	1
-1	1	0	-1
0	0	0	0
1	-1	0	1

dopant

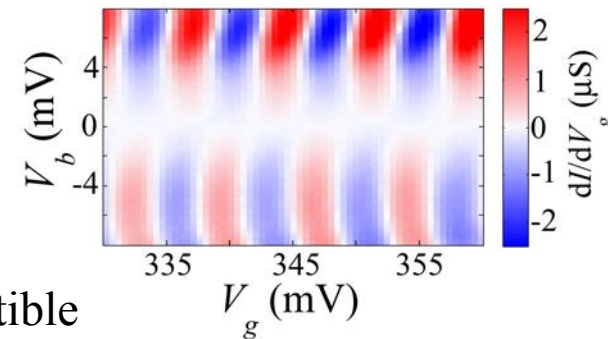


transconductance map



$$\frac{dI}{dV_g}$$

QD



fully CMOS compatible  
read out procedure

G. P. Lansbergen, M. Klein, S. Rogge, R. D. Levine and F. Remacle. Applied Physics Letters 2010, **96**, 043107

## Scheme for the balanced ternary addition

a  $n$  trit number,  $t_n t_{n-1} \dots t_0$  corresponds to the decimal number  $d$ :  $d = \sum_{i=0}^n t_i 3^i$

$$\text{addition : } d = x + y + z \quad \begin{cases} t_{carry} = \lfloor d/3 \rfloor \\ t_{sum} = d - t_{carry} \cdot 3 \end{cases}$$

$z = -1$

$z = 0$

$z = 1$

sum	<u>1</u>	0	1
1	1	0	1
0	1	1	0
1	0	1	1



sum	<u>1</u>	0	1
1	0	1	1
0	1	0	1
1	1	1	0



sum	<u>1</u>	0	1
1	1	1	0
0	0	1	1
1	1	0	1

carry	<u>1</u>	0	1
1	0	0	0
0	1	0	0
1	1	1	0



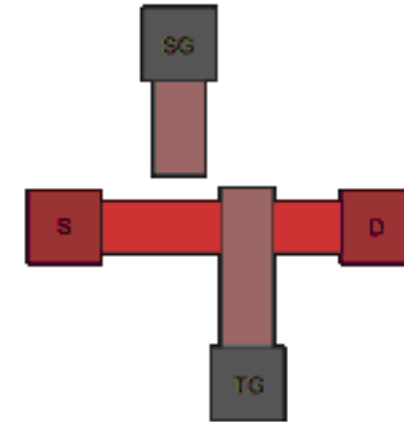
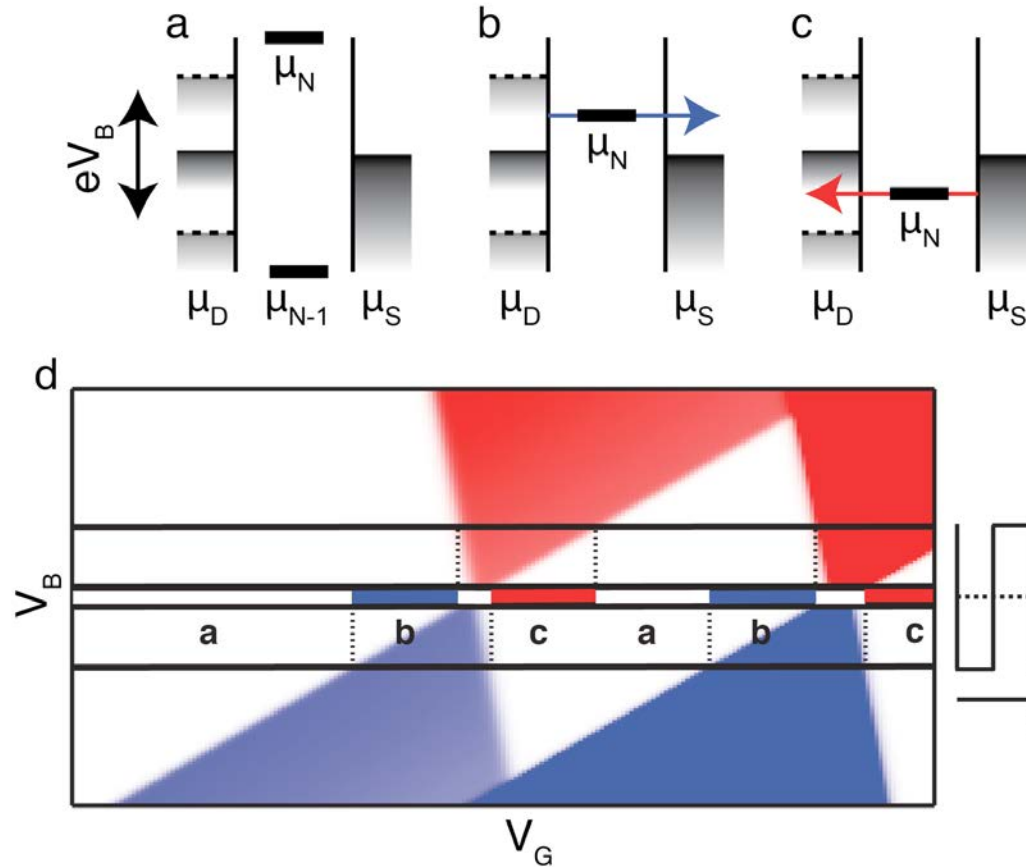
carry	<u>1</u>	0	1
1	0	0	1
0	0	0	0
1	1	0	0



carry	<u>1</u>	0	1
1	0	1	1
0	0	0	1
1	0	0	0



# Full ternary adder on a MOSSET device Metal on insulator SET

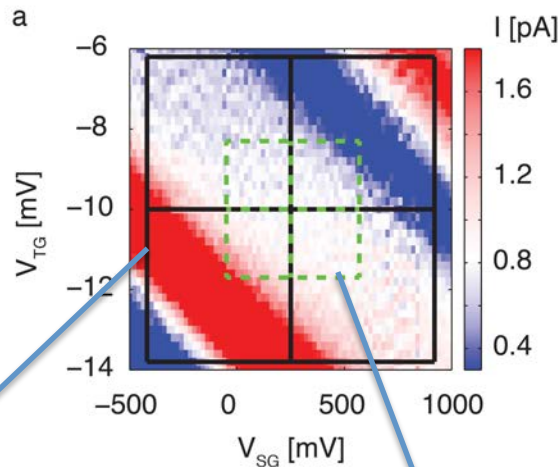
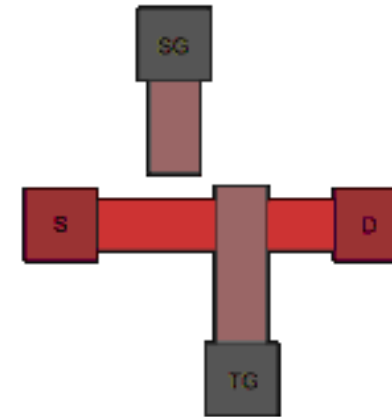


three gates : top, side and back gate

for the top and the side gate :  
applying an alternating (AC)  $V_B$  leads to negative, nul or positive current.

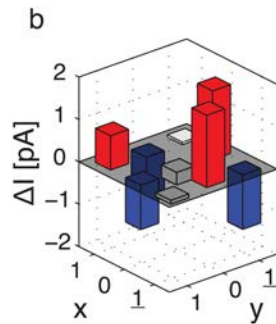
J. A. Mol, J. v. d. Heijden, J. Verduijn, M. Klein, F. Remacle, and S. Rogge, Appl. Phys. Lett., 99, 263109, 2011.

# Balanced ternary adder

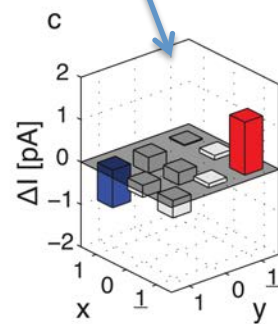


$x$  and  $y$  are mapped to the top and the side gates.  
 $z$  is mapped in the value of the back gate

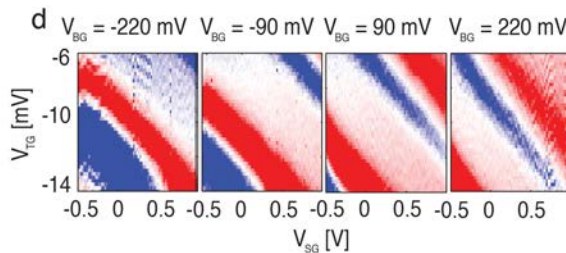
reading of the negative of the sum



reading of the negative of the carry out



changing the value of the back gate



- cascadable
- scalable
- process three ternary numbers
- inherently ternary

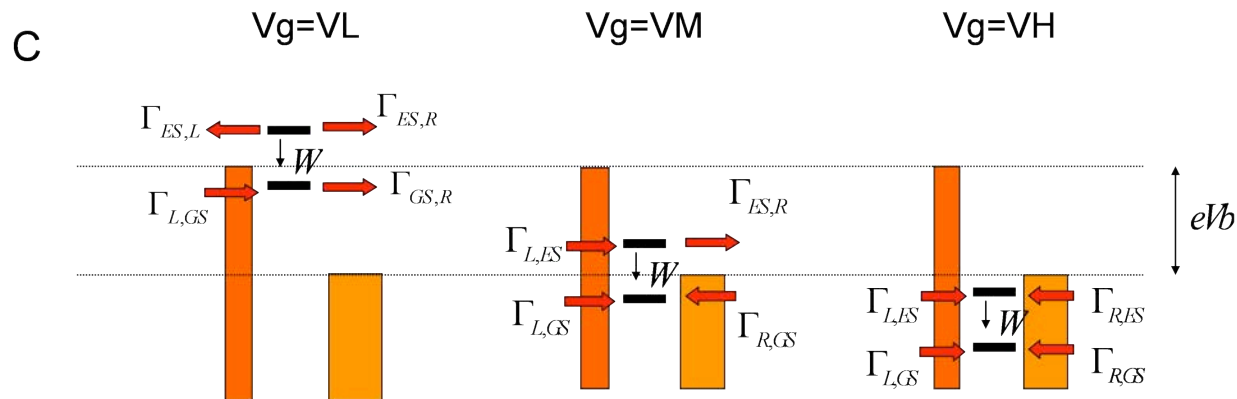
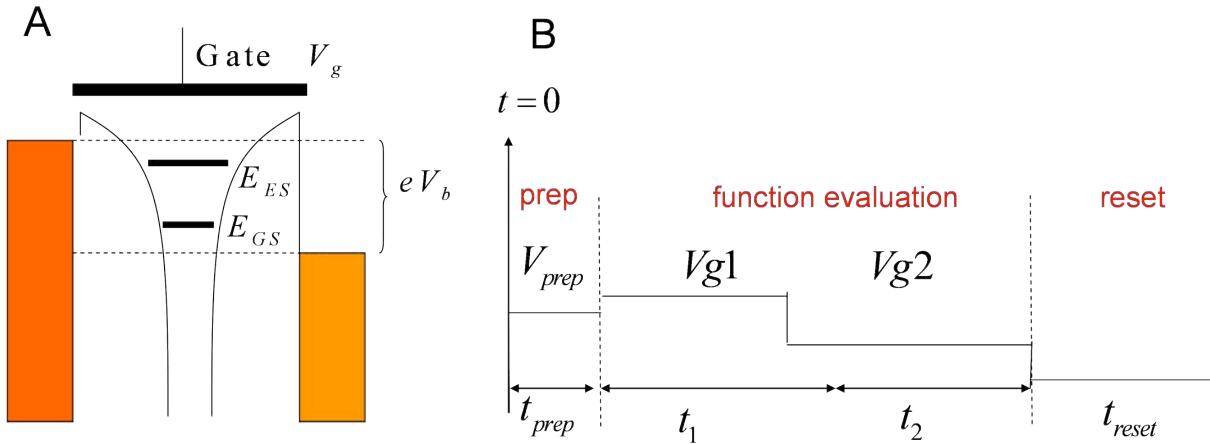
## Implementing a search algorithm addressing a SAT with a pulsed gate voltage

Aim : identifying one of the four functions of one bit

x	$F_1(x)$	$F_2(x)$	$F_3(x)$	$F_4(x)$
0	0	1	0	1
1	0	1	1	0

Using a quasiclassical algorithm, we can identify which function of one bit has been computed (by the Oracle) by the oracle in one query.

B. Fresch, J. Verduijn, J. A. Mol, S. Rogge, and F. Remacle, 2012, submitted



## Kinetic description of the relaxation between the two states

$$\mathbf{P} = \{P_{GS}, P_{ES}, P_0\} \quad P_0 = 1 - P_{GS} - P_{ES}$$

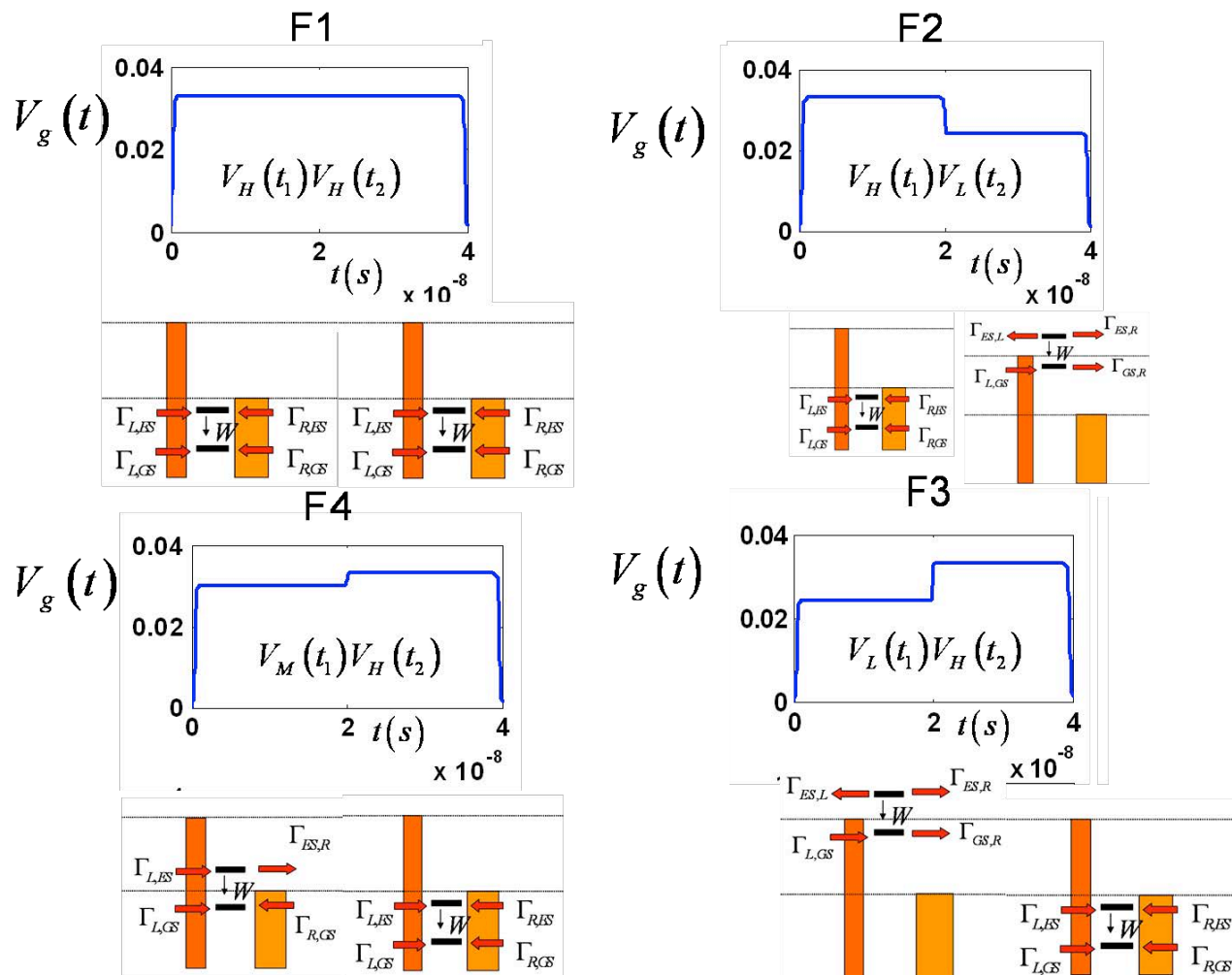
$$\mathbf{K}(t) = \begin{pmatrix} -(\Gamma_{GS,R} + \Gamma_{GS,L}) & W & (\Gamma_{R,GS} + \Gamma_{L,GS}) \\ 0 & -(\Gamma_{ES,R} + \Gamma_{ES,L} + W) & (\Gamma_{R,ES} + \Gamma_{L,ES}) \\ (\Gamma_{GS,R} + \Gamma_{GS,L}) & (\Gamma_{ES,R} + \Gamma_{ES,L}) & -(\Gamma_{R,GS} + \Gamma_{L,GS} + \Gamma_{R,ES} + \Gamma_{L,ES}) \end{pmatrix}$$

$W$  : relaxation rate between the GS and the ES induced by coupling to the phonons

$$d\mathbf{P}(t)/dt = \mathbf{K}(t)\mathbf{P}(t)$$

one electron at the time on the SAT

## Four double pulse profile are used to encode the four functions



output : stationary current

$$\bar{I}(T) = |e| \langle n \rangle_T / T \quad T = t_{prep} + t_1 + t_2 + t_{reset}$$

$\langle n \rangle_T$  is the average number of electrons tunneling through the SAT during  $T$

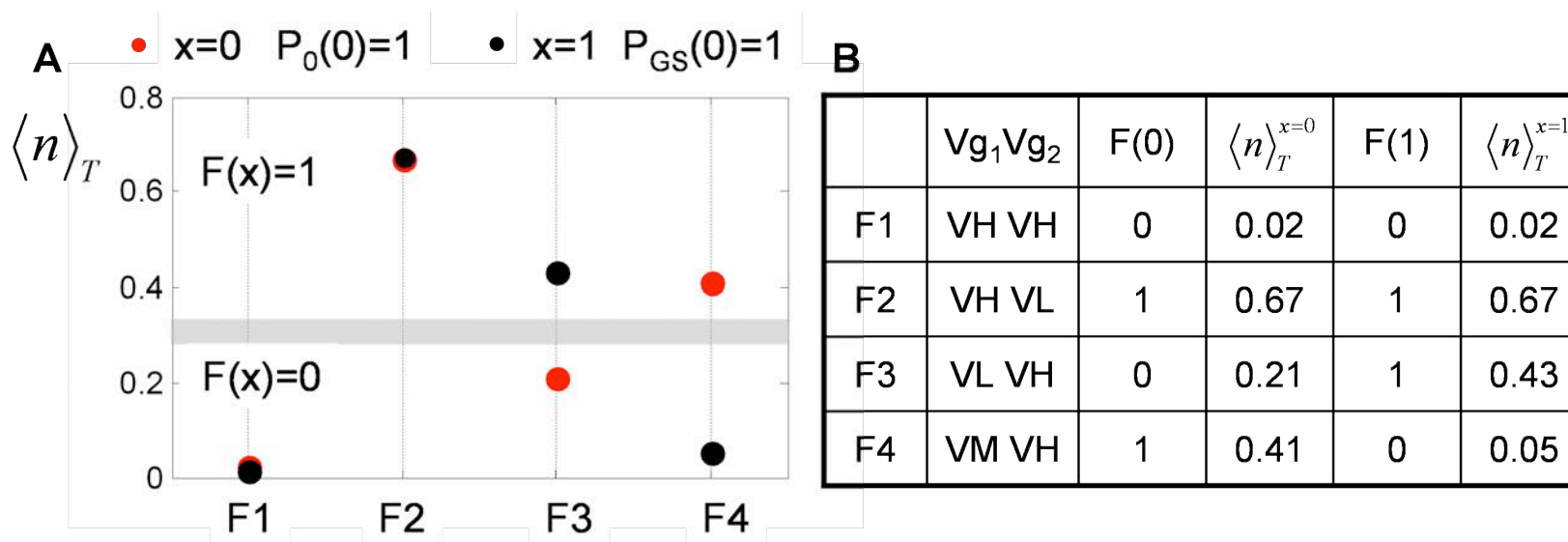
$$\begin{aligned} \langle n \rangle_T &= \int_0^{T-t_{reset}} \mathbf{\Gamma}(t) \cdot \mathbf{P}(t) dt + \langle n \rangle_{reset} \\ &= \int_0^{T-t_{reset}} dt \left( \Gamma_{GS,R}(t) P_{GS}(t) + \Gamma_{ES,R}(t) P_{ES}(t) \right) + \langle n \rangle_{reset} \end{aligned}$$

$$\mathbf{\Gamma}(t) \equiv (\Gamma_{GS,R}, \Gamma_{ES,R}, 0)$$

## Computing the four functions

$x = 1 \rightarrow P_{GS}(0) = 1$  realized by applying  $V_g = V_H$  for  $t_{prep}$

$x = 0 \rightarrow P_0(0) = 1$  realized by applying by applying  $V_L$  to empty the dot



Purely classical identification scheme requires two queries



## one query identification using a quasiclassical scheme

Prepare an initial probability vector that is a superposition of  $P_{GS}$  and  $P_0$

$$\text{canonical basis : } \mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \mathbf{e}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \begin{pmatrix} P_{GS} \\ P_{ES} \\ P_0 \end{pmatrix}$$

$$\mathbf{P}(0) = c_1 \mathbf{e}_1 + c_3 \mathbf{e}_3 \equiv c_1 [x=1] + c_3 [x=0]$$

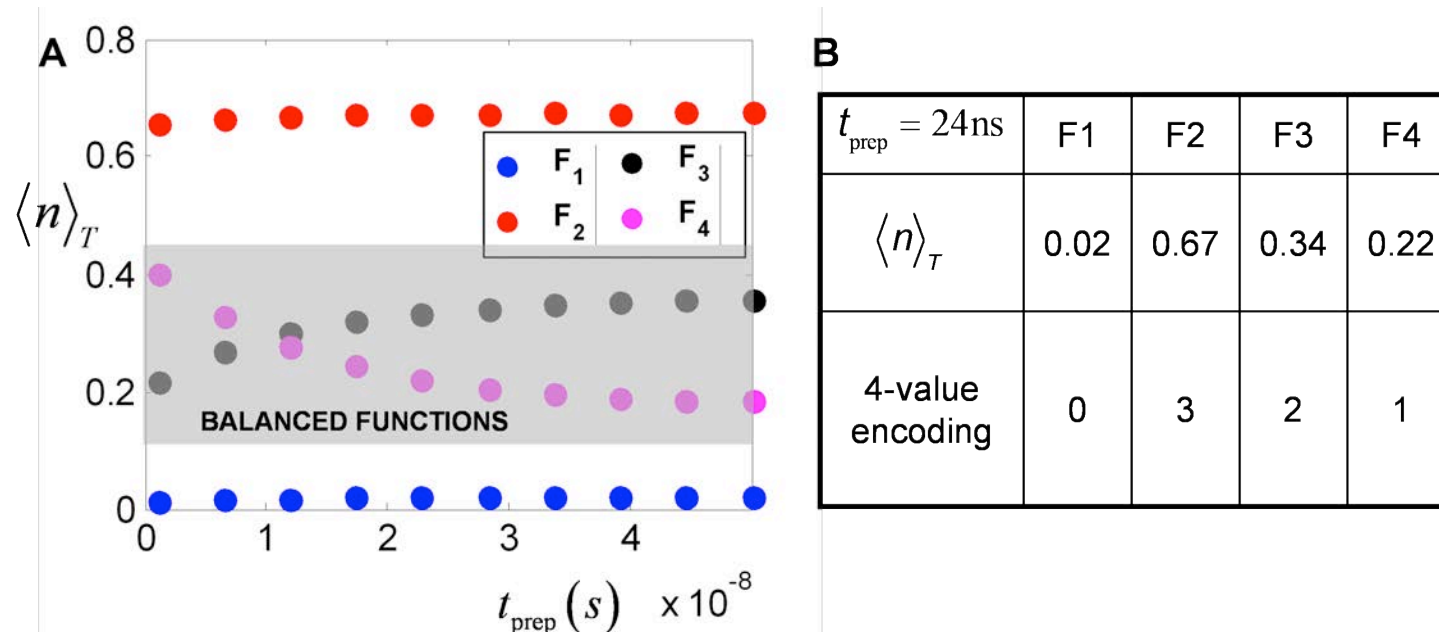
The kinetic scheme is linear, the general solution is

$$\mathbf{P}(t) = \mathbf{\Pi}(t) \mathbf{c} \quad \mathbf{\Pi}(t) = [\mathbf{e}_1(t), \mathbf{e}_2(t), \mathbf{e}_3(t)]$$

$$\text{The output is linear too } \langle n \rangle_T = c_1 \langle n \rangle_T^{x=1} + c_3 \langle n \rangle_T^{x=0}$$

using a superposition, one can in one query

- solve the Deutsch problem : is the function balanced or constant ?
- identify the function : one out of 4 possibilities



# Concluding remarks

- Multi-valued variables are inherent to the molecular and nanoscale.
- SAT's are CMOS compatible (no problem with undefined contact, interfacing with the macroscopic world).
- Atomic scale deterministic doping allows to reduce the variability problem.
- Quasiclassical parallelism can be implemented in the solid state using pulsed gate voltages.